IsobutyImalonic acid 4361-06-2 | DTXSID60195885

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Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.04

Global applicability domain: Outside

Local applicability domain index: 5.36e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

Image not found

2,6-Naphthalenedicarboxylic

acid

Measured: 6.46 Predicted: 4.10